On the Extremal Points of a Class of Polytopes of Matrices

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ABSTRACT

Let $\mathcal{M}_s(\mathbf{x}) := \{\mathbf{A} \in \Re^{n\times n} : \mathbf{A} \geqslant 0, \mathbf{A}^t = \mathbf{A}, \mathbf{Ae} = \mathbf{x}\}$, where $\mathbf{x}$ is a vector with positive entries. We show that an extremal point of $\mathcal{M}_s(\mathbf{x})$ can be written as the average between an extremal point of $\mathcal{M}(\mathbf{x}) := \{\mathbf{A} \in \Re^{n\times n} : \mathbf{A} \geqslant 0, \mathbf{Ae} = \mathbf{x}, \mathbf{A}^t\mathbf{e} = \mathbf{x}\}$ and its transpose. We then use this to characterize the vectors $\mathbf{x}$ that maximize the number of extremal points of $\mathcal{M}_s(\mathbf{x})$. Finally, we give a lower bound for the maximum number of extremal points of $\mathcal{M}_s(\mathbf{x})$.

1. INTRODUCTION

Let $\mathcal{M}_s(\mathbf{x}) := \{\mathbf{A} \in \Re^{n\times n} : \mathbf{A} \geqslant 0, \ \mathbf{A}^t = \mathbf{A}, \ \mathbf{Ae} = \mathbf{x}\}$ and $\mathcal{M}(\mathbf{x}) := \{\mathbf{A} \in \Re^{n\times n} : \mathbf{A} \geqslant 0, \mathbf{Ae} = \mathbf{x}, \mathbf{A}^t\mathbf{e} = \mathbf{x}\}$, where $\mathbf{x}$ is a vector with positive entries and $\mathbf{e}$ is the vector with all entries equal to 1. Then $\mathcal{M}_s(\mathbf{x})$ and $\mathcal{M}(\mathbf{x})$ are polytopes, and $\mathcal{M}_s(\mathbf{x})$ is a proper subset of $\mathcal{M}(\mathbf{x})$. Our primary interest is in the extremal points of $\mathcal{M}_s(\mathbf{x})$.

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Our first question is whether there is a relation between the extremal points of $\mathcal{M}_s(\mathbf{x})$ and the extremal points of $\mathcal{M}(\mathbf{x})$. It has been shown by Katz [3] and Cruse [2] that the answer is affirmative in the case $\mathbf{x} = \mathbf{e}$, that is, when the matrices are doubly stochastic. They showed that an extremal point of $\mathcal{M}_s(\mathbf{e})$ can be written as the average between an extremal point of $\mathcal{M}(\mathbf{e})$ and its transpose. In this paper, we show that this result is true in general.

The next question concerns the number of extremal points of $\mathcal{M}_s(\mathbf{x})$. To be specific, we want to characterize the vectors $\mathbf{x}$ that maximize the number of extremal points of $\mathcal{M}_s(\mathbf{x})$ and to give a lower bound on this number. This is a typical question that has been asked for $\mathcal{M}(\mathbf{x})$ and some other matrix polytopes. In fact, two recent papers by Kravtsov [4] and Loewy, Shier, and Johnson [5] answer the question for $\mathcal{M}(\mathbf{x})$. We combine our result on the relation between the extremal points of $\mathcal{M}_s(\mathbf{x})$ and $\mathcal{M}(\mathbf{x})$ with the techniques employed in these two papers to obtain an answer for $\mathcal{M}_s(\mathbf{x})$.

2. DEFINITIONS AND NOTATION

First, some matrix and vector notation. We denote matrices with bold uppercase letters and vectors with bold lowercase letters. The (i, j)th entry of a matrix $\mathbf{A}$ is denoted with a_{ij}, while the ith entry of vector $\mathbf{x}$ is denoted with x_i. We use $\langle n \rangle$ as shorthand for the set $\{1, 2, \dots, n\}$. Let $I \subseteq \langle n \rangle$. We use x_I as shorthand for $\sum_{i \in I} x_i$. Summation over an empty set is defined as zero. We reserve the letters $\mathbf{e}$ and $\hat{\mathbf{e}}$ for the vectors $(1, 1, \dots, 1)$ and $(n, n, \dots, n)$, respectively. We denote with $\mathbf{C}_k$ the fundamental $k \times k$ circulant matrix, i.e., the matrix with entries $c_{ij} = 1$ if $i = j + 1 \bmod k$, and $c_{ij} = 0$ otherwise.

In this paper, we deal only with undirected graphs. We allow *loops*, i.e., edges of the form (i, i), but we do not allow multiple edges. The *distance* between vertices i and j is defined as 0 if $i = j$, and as the minimum number of edges needed to traverse from i to j otherwise. A component of a graph always means a connected component. We define a *simple cactus*, or simply *cactus*, as a connected graph that can be obtained by adding an edge to a tree. Notice that a simple cactus contains exactly one cycle. A *simple odd cactus* is a simple cactus whose cycle's length is odd. A simple cactus whose cycle is a loop is called a *looped tree*. A *spike* of a simple cactus is a maximal connected subgraph of the cactus that does not contain an edge from the cactus's cycle. A spike, therefore, is a tree.

Let $\mathbf{A} \in \mathfrak{R}^{n \times n}$. We associate $\mathbf{A}$ with a bipartite graph with vertices i_r, i_c, $1 \leqslant i \leqslant n$, and edges (i_r, j_c), for every i, j such that $a_{ij} \neq 0$. We call such bipartite graph a *bipartite representation* of $\mathbf{A}$ and denote it with BG(A). We also associate $\mathbf{A}$ with a graph with vertices i, $1 \leqslant i \leqslant n$, and edges (i, j), for every i, j such that $a_{ij} \neq 0$ or $a_{ji} \neq 0$. We call such graph a *symmetric representation* of $\mathbf{A}$ and denote it with $G(\mathbf{A})$.

Let G be a graph with vertices i, $1 \leqslant i \leqslant n$ [i_r, i_c, $1 \leqslant i \leqslant n$, respectively], and $\mathscr{A}$ be a collection of $n \times n$ matrices. We say that G is *realizable* in $\mathscr{A}$ if $G = G(\mathbf{A})$ [$G = BG(\mathbf{A})$, respectively] for some $\mathbf{A} \in \mathscr{A}$. We call $\mathbf{A}$ a *realization* of G in $\mathscr{A}$.

We call the argument of $\mathscr{M}(\cdot)$ or $\mathscr{M}_s(\cdot)$ a *line-sum vector*, and we always assume it is a vector with positive entries. We denote with $\mathscr{E}(\mathbf{x})$ the set of all extremal points of $\mathscr{M}(\mathbf{x})$. An extremal point of a polytope is an element of the polytope that is not a convex combination of two distinct elements of the polytope. Similarly, we denote with $\mathscr{E}_s(\mathbf{x})$ the set of all extremal points of $\mathscr{M}_s(\mathbf{x})$. We define $D(\mathbf{x}) := \{\{I, J\} : \varnothing \neq I, J \subseteq \langle n \rangle,\ I \cap J = \varnothing,\ x_I = x_J\}$. A line-sum vector $\mathbf{x}$ is *k-degenerate* if $|D(\mathbf{x})| = k$. We also use the term *nondegenerate* for 0-degenerate. Let $\mathbf{x}, \mathbf{y}$ be line-sum vectors. A *spectrum* between $\mathbf{x}$ and $\mathbf{y}$, denoted with $S(\mathbf{x}, \mathbf{y})$, is defined as $S(\mathbf{x}, \mathbf{y}) := \{\lambda \in (0,1) : D(\mathbf{x}^\lambda) \neq \varnothing\}$, where $\mathbf{x}^\lambda := \lambda \mathbf{x} + (1 - \lambda)\mathbf{y}$. A spectrum $S(\mathbf{x}, \mathbf{y})$ is *simple* if $|D(\mathbf{x}^\lambda)| = 1$ for every $\lambda \in S(\mathbf{x}, \mathbf{y})$. Two polytopes $\mathscr{M}_s(\mathbf{x}), \mathscr{M}_s(\mathbf{y})$ are *equivalent* if

(1) for every $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$ there is a $\mathbf{B} \in \mathscr{E}_s(\mathbf{y})$ such that $G(\mathbf{B}) = G(\mathbf{A})$, and
(2) for every $\mathbf{B} \in \mathscr{E}_s(\mathbf{y})$ there is an $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$ such that $G(\mathbf{A}) = G(\mathbf{B})$.

Occasionally, we will apply a definition designed for a line-sum vector to polytopes, and vice versa. No confusion will arise here. Finally, we define $R(\mathbf{x}, \mathbf{y}) := \{\mathbf{A} \in \mathscr{E}_s(\mathbf{x}) : G(\mathbf{A}) \text{ is not realizable in } \mathscr{E}_s(\mathbf{y})\}$.

3. A RELATION BETWEEN THE EXTREMAL POINTS OF $\mathscr{M}_S(\mathbf{x})$ AND $\mathscr{M}(\mathbf{x})$

Katz [3] and Cruse [2] showed that an extremal point of the polytope of all symmetric, doubly stochastic matrices can be written as an average between a permutation matrix and its transpose. It is well known that the extremal points of the polytope of all doubly stochastic matrices are precisely the permutation matrices.

In this section, we extend their result by showing that, for any given line-sum vector $\mathbf{x}$, an extremal point of $\mathscr{M}_s(\mathbf{x})$ can be written as an average between an extremal point of $\mathscr{M}(\mathbf{x})$ and its transpose. Our arguments are solely graph-theoretic. We rely on the following theorem [1, Theorem 3.1] that characterizes the symmetric representation of an extremal point of $\mathscr{M}_s(\mathbf{x})$.

THEOREM 1. *Let* $\mathbf{A} \in \mathscr{M}_s(\mathbf{x})$. *Then the following are equivalent*:

(i) $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$,
(ii) *the components of* $G(\mathbf{A})$ *are trees or simple odd cacti*,
(iii) $\mathbf{A}$ *is the unique realization of* $G(\mathbf{A})$ *in* $\mathscr{M}_s(\mathbf{x})$.

Considering the way we obtain the entries of $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$, given $G(\mathbf{A})$ with only tree or simple odd cactus components, as suggested in the proof of Theorem 3.1 in [1], we have that

$$a_{ij} = \begin{cases} \frac{1}{2}(x_I - x_J) & \text{if } (i,j) \text{ is in a nonloop cycle,} \\ x_I - x_J & \text{otherwise} \end{cases}$$

for some $I, J \subseteq \langle n \rangle$, $I \neq \varnothing$, $I \cap J = \varnothing$. We also remark that given a line-sum vector $\mathbf{x}$ and a graph G whose components are simple odd cacti, we can uniquely obtain a matrix $\mathbf{A}$ satisfying $G(\mathbf{A}) = G$, $\mathbf{A}^t = \mathbf{A}$, and $\mathbf{Ae} = \mathbf{x}$ in the same fashion. This matrix $\mathbf{A}$, however, need not be nonnegative.

Another result (see [1, Theorem 2.1]) that we will need is that a matrix $\mathbf{A} \in \mathscr{M}(\mathbf{x})$ is in $\mathscr{E}(\mathbf{x})$ if and only if $\mathrm{BG}(\mathbf{A})$ has only tree components.

Finally, we need the following

LEMMA 2. *Let* $\mathbf{A} \in \mathfrak{R}^{n \times n}$ *be symmetric. Then* $\mathrm{BG}(\mathbf{A})$ *is a cycle if and only if* $G(\mathbf{A})$ *is a cycle and n is odd*, $n > 1$.

Proof. First notice that, by the symmetry of $\mathbf{A}$, an edge of $G(\mathbf{A})$ corresponds to exactly two edges of $\mathrm{BG}(\mathbf{A})$, and an edge of $\mathrm{BG}(\mathbf{A})$ corresponds to exactly one edge of $G(\mathbf{A})$. Therefore, the number of edges of $\mathrm{BG}(\mathbf{A})$ is exactly twice the number of edges of $G(\mathbf{A})$.

Assume that $\mathrm{BG}(\mathbf{A})$ is a cycle. Then $\mathrm{BG}(\mathbf{A})$ has exactly $2n$ edges, and each of its vertices is adjacent to exactly two distinct vertices. Hence $n > 1$, and $G(\mathbf{A})$ has exactly n edges. We can reindex the rows and columns of $\mathbf{A}$ simultaneously so that $a_{ij} \neq 0$ if and only if $j = i - 1$ or $j = i + 1$, where addition and subtraction are taken modulo n. Then $G(\mathbf{A})$ contains the cycle $(1,2),(2,3),\ldots,(n-1,n),(n,1)$. Since this cycle already has n edges, $G(\mathbf{A})$ cannot have any other edge. Therefore, $G(\mathbf{A})$ is a cycle.

If n is even, then traversing $\mathrm{BG}(\mathbf{A})$—starting from row 1—we have the cycle $(1_r, 2_c),(3_r, 2_c),(3_r, 4_c),\ldots,((n-1)_r,(n-2)_c),((n-1)_r, n_c),(1_r, n_c)$. But since it has only n edges, this cycle cannot be $\mathrm{BG}(\mathbf{A})$, a contradiction. Hence $G(\mathbf{A})$ is a cycle whose length is odd and greater than 1.

Now assume that $G(\mathbf{A})$ is a cycle and $n > 1$ is odd. Then $G(\mathbf{A})$ has exactly n edges, and each of its vertices is adjacent to exactly two distinct vertices.

Hence BG(**A**) has exactly $2n$ edges. Again we can reindex the rows and columns of **A** simultaneously as in the "only if" part of this proof. Since n is odd and greater than 1, traversing BG(**A**)—starting from row 1—will result in the cycle $(1_r, 2_c), (3_r, 2_c), (3_r, 4_c), \dots, (n_r, (n-1)_c), (n_r, 1_c), (2_r, 1_c), \dots, ((n-1)_r, n_c), (1_r, n_c)$. Since this cycle already has $2n$ edges, BG(**A**) cannot have any other edge. Therefore, BG(**A**) is a cycle. ∎

We now state our main result.

THEOREM 3. *Let* $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$. *Then* $\mathbf{A} = \frac{1}{2}(\mathbf{B} + \mathbf{B}^t)$ *for some* $\mathbf{B} \in \mathscr{E}(\mathbf{x})$.

Proof. Without loss of generality, assume that $G(\mathbf{A})$ is connected. We will construct **B**.

Define $b_{ij} := 0$ whenever $a_{ij} = 0$. For (i, j) in a tree or in a spike of a cactus, and for (i, j) a loop, we define $b_{ij} = b_{ji} := a_{ij}$. If $G(\mathbf{A})$ is a tree or a looped tree, we have $\mathbf{B} = \mathbf{A}$, and as a consequence of Lemma 2, $\mathrm{BG}(\mathbf{B}) = \mathrm{BG}(\mathbf{A})$ contains no cycle; hence **B** is in $\mathscr{E}(\mathbf{x})$.

If $G(\mathbf{A})$ is a simple odd cactus with nonloop cycle, then to complete the construction we only need to define the entries of **B** that correspond to the edges of the cycle. So now, assume that $G(\mathbf{A})$ is a cycle of odd length $n > 1$. Reindex the rows and columns of **A** simultaneously so that $a_{ij} \neq 0$ if and only if $j = i - 1$ or $j = i + 1$, where addition and subtraction are taken modulo n, and so that $a_{1n} = a_{n1} = \min\{a_{ij} \neq 0\} =: \alpha$. Then $\mathbf{B} := \mathbf{A} - \alpha \mathbf{C}_n + \alpha \mathbf{C}_n^t$ will do the job. It is clear that $\mathbf{A} = \frac{1}{2}(\mathbf{B} + \mathbf{B}^t)$. Next, for every i, $\sum_j b_{ij} = \sum_j a_{ij} - \alpha \sum_j c_{ij} + \alpha \sum_j c_{ji} = \sum_j a_{ij} - \alpha + \alpha = x_i$. Similarly, $\sum_i b_{ij} = x_j$ for every j. Hence $\mathbf{B} \in \mathscr{M}(\mathbf{x})$. Notice that $b_{1n} = 0$. So BG(**B**) can be obtained from BG(**A**) by removing at least one edge $(1, n)$. Since, by Lemma 2, BG(**A**) is a cycle, BG(**B**) has only tree components. Therefore, $\mathbf{B} \in \mathscr{E}(\mathbf{x})$. ∎

As consequences of the theorem we have the following:

COROLLARY 4. *Let* $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$. *If the components of* $G(\mathbf{A})$ *are trees or looped trees, then* $\mathbf{A} \in \mathscr{E}(\mathbf{x})$.

COROLLARY 5. *Let* $\mathbf{A} \in \mathscr{E}_s(\mathbf{x})$ *and* $\mathbf{A} = \frac{1}{2}(\mathbf{B} + \mathbf{B}^t) = \frac{1}{2}(\hat{\mathbf{B}} + \hat{\mathbf{B}}^t)$, *where* $\mathbf{B}, \hat{\mathbf{B}} \in \mathscr{E}(\mathbf{x})$. *Then* $\hat{\mathbf{B}} = \mathbf{B}$ *or* $\hat{\mathbf{B}} = \mathbf{B}^t$.

The nontrivial part of this corollary is when $G(\mathbf{A})$ contains a cycle. Again, assume that $G(\mathbf{A})$ is a cycle of odd length. Notice that BG(**B**) can be obtained from BG(**A**) by removing some edges that correspond to smallest positive entries of **A**. Graphically, we did this by traversing through BG(**A**) in such a way that the first edge is an edge to be removed. As we traverse, we alternately subtract from and add to the corresponding entries of **A** the amount α to get the entries of **B**. The only other possible way to construct **B** is by reversing the order of adding and subtracting α. In this way, we get the transpose of the matrix **B** obtained previously.

COROLLARY 6. *Let* $\mathbf{B} \in \mathscr{E}(\mathbf{x})$. *Then* $\frac{1}{2}(\mathbf{B}+\mathbf{B}^t) \in \mathscr{E}_s(\mathbf{x})$ *if and only if the components of* $G(\mathbf{B})$, *the symmetric representation of* **B**, *and trees or simple odd cacti.*

4. LINE-SUM VECTOR THAT MAXIMIZES THE NUMBER OF EXTREMAL POINTS

Recently, Kravtsov [4] and Loewy, Shier, and Johnson [5] characterized line-sum vectors that maximize the number of extremal points of $\mathscr{M}(\mathbf{x})$. They showed that a line-sum vector $\tilde{\mathbf{x}}$ maximizes the number of extremal points of $\mathscr{M}(\mathbf{x})$ if and only if it satisfies the following two properties:

(a) (Nondegeneracy) $\tilde{x}_I = \tilde{x}_J$ only if $I = J$, and
(b) $\tilde{x}_I > \tilde{x}_J$ if $|I| > |J|$,

where $\varnothing \neq I, J \subseteq \langle n \rangle$.

Kravtsov also gave an example of such vectors,

$$\hat{\mathbf{x}} = \left(n + \frac{1}{2}, n + \frac{1}{2^2}, \ldots, n + \frac{1}{2^n} \right).$$

We call this vector the *Kravtsov vector*.

In this section, we will show that those line-sum vectors also maximize the number of extremal points of $\mathscr{M}_s(\mathbf{x})$. We will follow Kravtsov's approach very closely (see [4] and also [6, Chapter 6]).

Our first step is to show that a line-sum vector satisfying (a) always give more extremal points than ones that do not satisfy (a).

THEOREM 7. *Let* $\mathscr{M}_s(\mathbf{x})$ *be p-degenerate,* $p > 0$. *Then there exists an q-degenerate* $\mathscr{M}_s(\mathbf{y})$, $0 \leqslant q < p$, *such that* $|\mathscr{E}_s(\mathbf{y})| \geqslant |\mathscr{E}_s(\mathbf{x})|$, *where the equality holds only if* $n = 2$.

Proof. Let K, L be proper, disjoint subsets of $\langle n \rangle$ satisfying $x_K = x_L$, and $P = (K \cup L)'$. Assume that $|K| \geqslant |L|$.

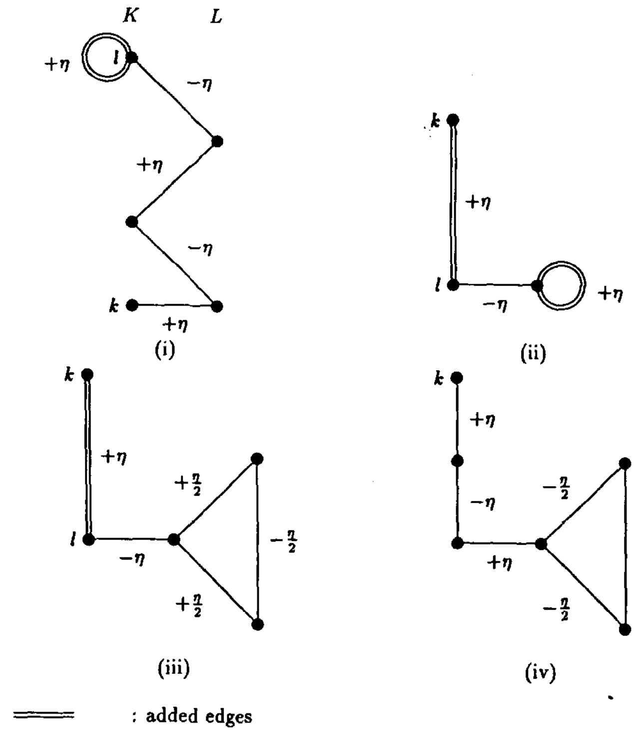

FIG. 1. Changes in entries of **A** to obtain the corresponding entries of **B** in the proof of Theorem 7.

Pick any $k \in K$, and define y by $y_k := x_k + \eta$, else $y_i := x_i$, where $\eta := \min_{A \in \mathscr{E}_s(\mathrm{x})} \min\{a_{ij} > 0\}$. Then $y_K > y_L$. Moreover, by the choice of η, $\{I, J\} \notin D(\mathrm{x})$ implies $\{I, J\} \notin D(\mathrm{y})$ for any pair of proper, disjoint subsets I, J of $\langle n \rangle$. Therefore, y is q-degenerate, $0 \leqslant q < p$.

Next, we construct a 1-1 mapping from $\mathscr{E}_s(\mathrm{x})$ into $\mathscr{E}_s(\mathrm{y})$. Let $A \in \mathscr{E}_s(\mathrm{x})$. We have three cases.

Case I. $a_{ij} = 0$ *for all* $(i, j) \in (K' \times L) \cup (K \times L')$. Then one component of $G(A)$ is a connected bipartite tree with parts K and L. We may map **A** to a $\mathbf{B} \in \mathscr{E}_s(\mathrm{y})$ in either of the following ways:

(i) Pick any $l \in K$. We construct **B** via $G(\mathbf{B})$ which is obtained by adding to $G(\mathbf{A})$ a loop at l. The possibility of such construction is illustrated in Figure 1(i).

(ii) Pick any $l \in P$. We construct **B** via $G(\mathbf{B})$ which is obtained by adding to $G(\mathbf{A})$ the edge (k, l) and, if the component containing l does not have a cycle, also a loop at a first neighbor of l. The possibilities of such constructions are illustrated in Figure 1(ii) and (iii).

Case II. $a_{kk} > 0$. Then we map $\mathbf{A}$ to $\mathbf{B} \in \mathscr{E}_s^c(\mathbf{y})$ defined by $b_{kk} := a_{kk} + \eta$, else $b_{ij} := a_{ij}$. In this case we have $G(\mathbf{B}) = G(\mathbf{A})$.

Case III. $a_{kk} = 0$, *but* $a_{ij} > 0$ *for some* $(i, j) \in (K' \times L) \cup (K \times L')$. We map $\mathbf{A}$ to $\mathbf{B} \in \mathscr{E}_s^c(\mathbf{y})$ constructed via $G(\mathbf{B})$ as follows:

(i) if the component containing k does not have a cycle, then obtain $G(\mathbf{B})$ by adding to $G(\mathbf{A})$ a loop at k;

(ii) otherwise, take $G(\mathbf{B}) = G(\mathbf{A})$.

The possibility of the latter construction is illustrated in Figure 1(iv).

By considering their symmetric representations, it is not difficult to show that the matrices $\mathbf{B}$ constructed above all are distinct, establishing the existence of a 1-1 mapping from $\mathscr{E}_s^c(\mathbf{x})$ into $\mathscr{E}_s^c(\mathbf{y})$. Also, for $n \geqslant 3$, by virtue of case I, the map cannot be onto. ■

As a consequence, a line-sum vector gives a maximum number of extremal points only if it is nondegenerate. We remark that the symmetric representation of an extremal point with a nondegenerate line-sum vector has only simple odd cactus components.

Next, we show that among nondegenerate line-sum vectors, the ones that also satisfy (b) have the most extremal points. Recall [4, Theorems 1, 1′] that these vectors are precisely the nondegenerate line-sum vectors whose spectrums with $\hat{\mathbf{e}}$ are empty. We need a lemma.

LEMMA 8. *Let* $\mathscr{M}_s(\mathbf{x}), \mathscr{M}_s(\mathbf{y})$ *be nondegenerate. Then there exists an* $\mathscr{M}_s(\mathbf{z})$ *such that*:

(i) $\mathscr{M}_s(\mathbf{y})$ *and* $\mathscr{M}_s(\mathbf{z})$ *are equivalent, and*

(ii) $S(\mathbf{x}, \mathbf{z})$ *is simple.*

Proof. Follows from Lemma 2 of [4] and Theorem 2. ■

THEOREM 9. *Let* $\mathscr{M}_s(\mathbf{x})$ *be nondegenerate with simple, nonempty spectrum* $S(\mathbf{x}, \hat{\mathbf{e}})$. *Let* $\hat{\mathbf{y}} = \hat{\lambda}\mathbf{x} + (1 - \hat{\lambda})\hat{\mathbf{e}}$, $\hat{\lambda} \in (0, 1)$, *satisfy*:

(i) $\mathscr{M}_s(\hat{\mathbf{y}})$ *is nondegenerate, and*

(ii) $|S(\hat{\mathbf{y}}, \hat{\mathbf{e}})| = |S(\mathbf{x}, \hat{\mathbf{e}})| - 1$.

Then $|\mathscr{E}_s^c(\hat{\mathbf{y}})| \geqslant |\mathscr{E}_s^c(x)|$.

Proof. Let $\hat{\mathbf{y}}$ be as described in the theorem. Then the spectrum $S(\hat{\mathbf{y}}, \hat{\mathbf{e}})$ is simple.

Let $\mathbf{x}^\lambda$ denote $\lambda\mathbf{x}+(1-\lambda)\hat{\mathbf{e}}$.

Let $\lambda_1 := \max\{\lambda \in S(\mathbf{x}, \hat{\mathbf{e}})\}$. Then, by (ii), $\lambda_1 > \hat{\lambda}$. Let $D(\mathbf{x}^{\lambda_1}) = \{\{K, L\}\}$. Notice that $\mu(\mathbf{x}^\lambda) := x_K^\lambda - x_L^\lambda$ is a linear function of λ, and that $\mu(\mathbf{x}^{\lambda_1}) = 0$. Without loss of generality, assume $\mu(\mathbf{x}) < 0$. Then $\mu(\mathbf{x}^\lambda) > 0$ for $\lambda < \lambda_1$. Therefore $\mu(\hat{\mathbf{y}}) > 0$, and also $\mu(\mathbf{z}) > 0$, where $\mathbf{z} = \mathbf{x}^{\lambda^*}$ for some $\lambda^* \in (0,1)$, such that $\mathscr{M}_s(\mathbf{z})$ is nondegenerate and $S(\mathbf{z}, \hat{\mathbf{e}}) = \varnothing$. Since $\mathbf{z}$ satisfies (b), we have $|K| \geqslant |L|$.

Let $\mathbf{A} \in R(\mathbf{x}, \hat{\mathbf{y}})$, and $G := G(\mathbf{A})$. Let $\mathbf{B} \in \mathfrak{R}^{n \times n}$ satisfy $G(\mathbf{B}) = G$, $\mathbf{B}^t = \mathbf{B}$, and $\mathbf{Be} = \hat{\mathbf{y}}$. Since $G(\mathbf{B})$ has simple odd cactus components, $\mathbf{B}$ is unique. Since $G(\mathbf{B})$ is not realizable in $\mathscr{E}_s^c(\hat{\mathbf{y}})$, $b_{ij} = b_{ji} < 0$ for some (i,j). No other entry of $\mathbf{B}$ is negative; otherwise the corresponding entry of $\mathbf{A}$ would also be negative. There are three possible positions for edge (i,j) in G:

I. (i,j) is in a spike of a cactus,
II. (i,j) is a loop, i.e., $i=j$, and
III. (i,j) is in a nonloop cycle.

Notice that in cases I and II, $b_{ij} = \hat{y}_L - \hat{y}_K$, and $a_{ij} = x_L - x_K$, while in case III, $b_{ij} = \frac{1}{2}(\hat{y}_L - \hat{y}_K)$, and $a_{ij} = \frac{1}{2}(x_L - x_K)$.

Case I: Assume that j is farther from the cactus's cycle than i. The removal of (i,j) will split the cactus containing (i,j) into two components: one contains i, and the other contains j. Let S be the set of all vertices in the component that contains j. Then $K = \{k \in S : \text{distance between } k \text{ and } j \text{ is odd}\}$, and $L = \{k \in S : \text{distance between } k \text{ and } j \text{ is even}\}$. For $k \in S$, obtain a graph $G(k)$ from G by replacing edge (i,j) with edge (i,k). Then $G(k)$ is realizable in $\mathscr{E}_s^c(\hat{\mathbf{y}})$ but not in $\mathscr{E}_s^c(\mathbf{x})$ whenever $k \in K$, and $G(k)$ is realizable in $\mathscr{E}_s^c(\mathbf{x})$ but not in $\mathscr{E}_s^c(\hat{\mathbf{y}})$ whenever $k \in L$. In this case, we obtain $|K|$ elements of $R(\hat{\mathbf{y}}, \mathbf{x})$, and $|L|$ elements of $R(\mathbf{x}, \hat{\mathbf{y}})$.

Case II: Let S be the set of all vertices in the component containing $i = j$. Then $K = \{k \in S : \text{distance between } k \text{ and } i \text{ is odd}\}$, and $L = \{k \in S : \text{distance between } k \text{ and } i \text{ is even}\}$. Consider the following two ways of obtaining other graphs from G:

(i) Replace the loop at i with a loop at $k \in S$ to obtain $G(k)$. Then $G(k)$ is realizable in $\mathscr{E}_s^c(\hat{\mathbf{y}})$ but not in $\mathscr{E}_s^c(\mathbf{x})$ whenever $k \in K$, and $G(k)$ is realizable in $\mathscr{E}_s^c(\mathbf{x})$ but not in $\mathscr{E}_s^c(\hat{\mathbf{y}})$ whenever $k \in L$.

(ii) Replace the loop at i with an edge connecting two distinct vertices k,l, both of which are either in K or in L, to obtain $G(k,l)$. Then $G(k,l)$ is realizable in $\mathscr{E}_s^c(\hat{\mathbf{y}})$ but not in $\mathscr{E}_s^c(\mathbf{x})$ whenever $k,l \in K$, and $G(k,l)$ is realizable in $\mathscr{E}_s^c(\mathbf{x})$ but not in $\mathscr{E}_s^c(\hat{\mathbf{y}})$ whenever $k,l \in L$.

In this case, we obtain $\frac{1}{2}|K|(|K|+1)$ elements of $R(\hat{\mathbf{y}},\mathbf{x})$, and $\frac{1}{2}|L|(|L|+1)$ elements of $R(\mathbf{x},\hat{\mathbf{y}})$.

Case III: This case is a dual of case II. Both i,j are in L. We replace edge (i,j) with either a loop or an edge connecting two distinct vertices in the same subset K or L. We then have the same numbers as in case II.

What we have shown is that we can partition $R(\mathbf{x},\hat{\mathbf{y}})$ and $R(\hat{\mathbf{y}},\mathbf{x})$ so that there is a 1-1 mapping from the set of all partition classes of $R(\mathbf{x},\hat{\mathbf{y}})$ onto the set of all partition classes of $R(\hat{\mathbf{y}},\mathbf{x})$ with the property that the cardinality of each partition class of $R(\mathbf{x},\hat{\mathbf{y}})$ is not greater than the cardinality of its map. We have, therefore, $|\mathscr{E}_s(\hat{\mathbf{y}})| \geqslant |\mathscr{E}_s(\mathbf{x})|$. ∎

Combining Theorems 7 and 9, we conclude that a line-sum vector $\tilde{\mathbf{x}}$ maximizes the number of extremal points of $\mathscr{M}_s(\mathbf{x})$ only if $\tilde{\mathbf{x}}$ satisfies conditions (a) and (b). The converse is also true. We prove it by showing that if $\mathbf{x},\mathbf{y}$ are line-sum vectors satisfying (a) and (b), then $|\mathscr{E}_s(\mathbf{x})| = |\mathscr{E}_s(\mathbf{y})|$.

By Lemma 8, we may assume that $S(\mathbf{x},\mathbf{y})$ is simple. Let the elements of $S(\mathbf{x},\mathbf{y})$ be $\lambda_1 > \lambda_2 > \cdots > \lambda_m$. Let $\mathbf{z} = \lambda\mathbf{x}+(1-\lambda)\mathbf{y}$, $\lambda_1 > \lambda > \lambda_2$. Let $D(\lambda_1\mathbf{x}+(1-\lambda_1)\mathbf{y}) = \{\{K,L\}\}$, and assume $x_K - x_L < 0$. Then $y_K - y_L > z_K - z_L > 0$. Since both $\mathbf{x}$ and $\mathbf{y}$ satisfy (b), we have $|K| = |L|$. Since $x_I - x_J$ and $z_I - z_J$ have different signs only if $\{I,J\} = \{K,L\}$, $\mathbf{z}$ must satisfy (b). We then proceed, as in the proof of Theorem 9, to partition $R(\mathbf{x},\mathbf{z})$ and $R(\mathbf{z},\mathbf{x})$ and construct a 1-1 mapping from the set of all partition classes of $R(\mathbf{x},\mathbf{z})$ onto the set of all partition classes of $R(\mathbf{z},\mathbf{x})$. This time, however, the cardinality of a partition class of $R(\mathbf{x},\mathbf{z})$ equals the cardinality of its map. Hence $|\mathscr{E}_s(\mathbf{x})| = |\mathscr{E}_s(\mathbf{z})|$. Repeating this inductively, we have $|\mathscr{E}_s(\mathbf{x})| = |\mathscr{E}_s(\mathbf{y})|$.

This establish the following

THEOREM 10. *A line-sum vector* $\tilde{\mathbf{x}}$ *maximizes* $|\mathscr{E}_s(\mathbf{x})|$ *if and only if* $\tilde{\mathbf{x}}$ *satisfies* (a) *and* (b).

5. A LOWER BOUND FOR THE MAXIMUM NUMBER OF EXTREMAL POINTS

In this section, we will give a lower bound for the number of extremal points of $\mathscr{M}_s(\mathbf{x})$, where $\mathbf{x}$ is a maximizing line-sum vector. We obtain this bound by counting all extremal points from two sources: ones whose symmetric representation contains a cycle of the largest possible length, and ones whose symmetric representation has only looped-tree components. It will be convenient to take $\hat{\mathbf{x}}$, the Kravtsov vector, as the maximizing line-sum vector being considered. Notice that for $\varnothing \neq I, J \subseteq \langle n \rangle$, $I \cap J = \varnothing$, $|I| = |J|$, we have $\hat{x}_I > \hat{x}_J$ if and only if $\min\{i \in I\} > \min\{j \in J\}$.

We work first on extremal points whose symmetric representation contains a cycle of the largest possible length.

Consider first the case when n is odd. We claim that n is the largest possible length. In fact, we can construct an extremal point whose symmetric representation is any given cycle of length n by taking as its positive entries the entries of the vector $\frac{1}{2}(\sum_{k=0}^{n-1}(-1)^k C_n^k)\tilde{\mathbf{x}}$, where $\tilde{\mathbf{x}}$ is the appropriate rearrangement of $\hat{\mathbf{x}}$. Hence, when n is odd, there are $\frac{1}{2}(n-1)!$ extremal points whose symmetric representation contains a cycle of the largest possible length.

When n is even, a cycle of length n is not realizable in $\mathscr{E}_s(\hat{\mathbf{x}})$. We can construct an extremal point whose symmetric representation has a given cycle component of length $n-1$ by taking as its positive entries the entries of the vector $\frac{1}{2}(\sum_{k=0}^{n-2}(-1)^k C_{n-1}^k)\tilde{\mathbf{x}}$, where $\tilde{\mathbf{x}}$ is the appropriate rearrangement of $n-1$ entries of $\hat{\mathbf{x}}$. There are $\frac{1}{2}n(n-2)!$ such extremal points. We can also construct an extremal point whose symmetric representation is connected and contains a cycle of length $n-1$. However, this type of graph is realizable in $\mathscr{E}_s(\hat{\mathbf{x}})$ if and only if the vertex outside the cycle is adjacent to the vertex that corresponds to the largest line sum. There are $\frac{1}{2}(n-1)!$ such extremal points. Therefore, when n is even, there are $\frac{1}{2}(2n-1)(n-2)!$ extremal points whose symmetric representation contains a cycle of the largest possible length.

For extremal points whose symmetric representation has looped trees as its components, we will use a tool introduced by Loewy, Shier, and Johnson [5]. We call a graph with only tree components a *Loewy-Shier-Johnson graph*, or an *LSJ graph* for short, if its vertex set is $\{(i, \pi(i)) : 1 \leqslant i \leqslant n\}$, where π is a permutation on n objects, and each of its tree components satisfies the following two properties:

(i) $\bigcup i = \bigcup \pi(i)$, where the unions are taken over all vertices $(i, \pi(i))$ in the component, and

(ii) (Nonseparating property) removal of any edge in the component does not create a new component on which the relation $\bigcup i = \bigcup \pi(i)$ holds.

In their paper, Loewy et al. showed that each LSJ graph corresponds uniquely to an extremal point of $\mathscr{M}(\hat{\mathbf{x}})$, and vice versa.

By Corollary 4, an extremal point of $\mathscr{M}_s(\hat{\mathbf{x}})$ whose symmetric representation has only looped-tree components is also an extremal point of $\mathscr{M}(\hat{\mathbf{x}})$. Such an extremal point, therefore, corresponds uniquely to an LSJ graph. We will show that this corresponding LSJ graph has a special structure.

Let G be a symmetric representation of an extremal point of $\mathscr{M}_s(\hat{\mathbf{x}})$ whose components are looped trees, and G_1 be its corresponding LSJ graph. We state some rather obvious facts.

(1) If $(i, \pi(i))$ is a vertex in G_1, then $(i, \pi(i))$ is an edge in G.

(2) Two vertices i, j in G are connected if and only if the vertices $(i, \pi(i)), (j, \pi(j))$ are connected in G_1.

(3) No vertices (i, i) and (j, j) in G_1 may be connected.

(4) The permutation π is a product of disjoint (permutation) cycles of length 2 (transposition) or length 1 (fixed point).

We are now ready to describe the structure of G_1. For simplicity, we assume that G is connected, i.e., G itself is a looped tree.

Consider first the case when n is even. Then, from (3) and (4), π is a product of $n/2$ transpositions. These transpositions contribute to $n/2$ edges of G. Hence, the $n-1$ edges of G_1 contribute to the other $n/2$ edges of G. Notice that at most two edges of G_1 may contribute to one edge of G. It is not difficult to show that there is exactly one edge of G_1 that contributes singly to an edge of G. This edge of G_1 connects $(t, \pi(t))$ to $(\pi(t), t)$, where t is the looped vertex of G. Each of the other edges of G_1 connects $(i, \pi(i))$ to $(j, \pi(j))$, where $j \neq \pi(i)$, and the vertices of G_1 satisfy the following: $(i, \pi(i))$ and $(j, \pi(j))$ are adjacent if and only if $(\pi(i), i)$ and $(\pi(j), j)$ are also adjacent.

A more useful description of G_1 is as follows. G_1 is an LSJ graph that has exactly one edge connecting two vertices of the form $(i, \pi(i))$ and $(\pi(i), i)$, and removal of this edge splits G_1 into two subtrees that are *reflexive* to each other. By this we mean:

(i) if $(j, \pi(j))$ is in one subtree, then $(\pi(j), j)$ is in the other subtree, and

(ii) $(i, \pi(i))$ and $(j, \pi(j))$ are adjacent in one subtree if and only if $(\pi(i), i)$ and $(\pi(j), j)$ are also adjacent in the other subtree.

Conversely, given an LSJ graph G_1 with this structure and its corresponding matrix $\mathbf{A}$ in $\mathscr{E}(\mathbf{x})$, an edge of G_1 and its reflection both correspond to the same edge of $G(\mathbf{A})$. Using a counting argument, we have that $G(\mathbf{A})$ is a looped tree; therefore $\mathbf{A}$ is in $\mathscr{E}_s(\mathbf{x})$. Hence, an LSJ graph with this structure corresponds uniquely to a looped tree.

Figure 2 shows two examples of a looped tree and its corresponding LSJ graph for $n = 6$.

We conclude that given a permutation π as a product of $n/2$ disjoint transpositions, it corresponds to $n^{n/2-1}$ extremal points of $\mathscr{M}_s(\hat{\mathbf{x}})$ whose symmetric representation is a looped tree.

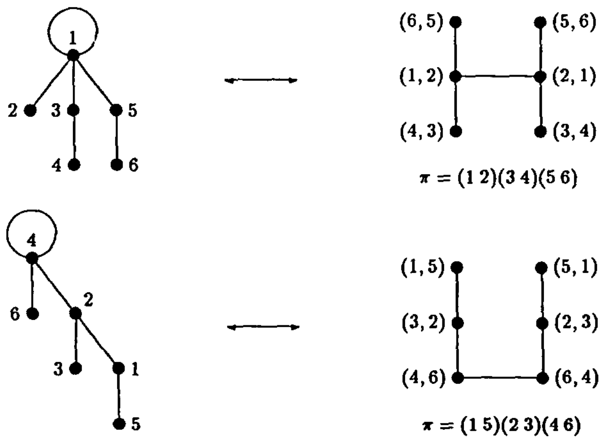

FIG. 2. Examples of looped trees and their corresponding LSJ graphs, $n = 6$.

Next we consider thē case when n is odd. From (3) and (4), π is a product of $(n-1)/2$ disjoint transpositions and one fixed point. These transpositions and fixed point contribute to $(n+1)/2$ edges of G. Hence, the $n-1$ edges of G_1 contribute to the other $(n-1)/2$ edges of G. It can be shown that no edge of G_1 contributes singly to an edge of G. Hence, each of the edges of G_1 connects $(i, \pi(i))$ to $(j, \pi(j))$, where $j \neq \pi(i)$, and its

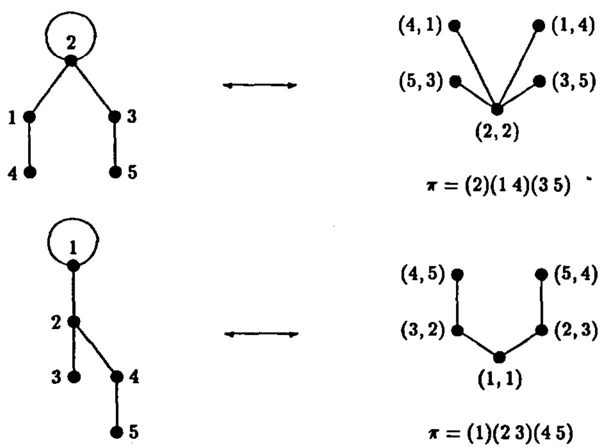

FIG. 3. Examples of looped trees and their corresponding LSJ graphs, $n = 5$.

TABLE 1

n	Number of extremal points		
	Looped-tree case	Largest-cycle case	Lower bound
3	7	1	8[a]
4	34	7	41[a]
5	236	12	248
6	1936	132	2068
7	19762	360	20122
8	204212	5400	209612

[a] Exact.

vertices satisfy the following: $(i, \pi(i))$ and $(j, \pi(j))$ are adjacent if and only if $(\pi(i), i)$ and $(\pi(j), j)$ are also adjacent.

We may also describe G_1 as follows. G_1 is an LSJ graph that can be obtained as a union of two reflexive subtrees whose intersection contains only a vertex of the form (i, i). As in the case n even, we can show that an LSJ graph with this structure corresponds uniquely to a looped tree.

Figure 3 shows two examples of a looped tree and its corresponding LSJ graph for $n = 5$.

Given a permutation π as a product of disjoint $(n-1)/2$ transpositions and one fixed point, it corresponds to $(n+1)^{(n-3)/2}$ extremal points of $\mathscr{M}_s(\hat{\mathbf{x}})$ whose symmetric representation is a looped tree.

Bounds for several n are given in Table 1.

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